INDIAN INSTITUTE OF INFORMATION TECHNOLOGY
DESIGN AND MANUFACTURING (IIITDM) KANCHEEPURAM

INTRODUCTION OF NEW COURSE

Course Title	**Atomistic Modeling of Materials**	Course Code	PHY5XXX			
Dept./ Specialization	Physics	Structure (LTPC)	3	1	0	4
To be offered for	UG/PG	Status	Core ☐		Elective ■	
Faculty Proposing the course	Dr. Debolina Misra	Type	New ■		Modification ☐	
Recommendation from the DAC		Date of DAC	04-02-2021			
External Expert(s)	Prof. Tarun Kundu (IIT Kharagpur), Prof. Satyesh Yadav (IIT Madras)					
Pre-requisite	Nil	Submitted for approval			45th Senate	
Learning Objectives	Focusing primarily on DFT-based calculations of materials properties, this course is intended to provide students from diverse backgrounds an overview of modeling materials at the basic of length scale namely the atomic scale.					
Learning Outcomes	After completion of this course students will be able to run DFT calculations. They will be able to design/model materials as a set of atoms in terms of molecular/bulk/surface structures for calculating their properties and predicting materials for specific device applications.					
Contents of the course *(With approximate break-up of hours for L/T/P)*	**Introduction:** Introduction to computational materials science: necessity and applications, crystals and symmetry, Crystal planes, Miller indices, theory of X-ray diffraction in brief, Reciprocal space, Brillouin zone (L12+T2) **Theory:** Evolution of density functional theory starting from basic quantum mechanics, Hatree-Fock equation, Slater determinant, Kohn-Sham equations. (L12) **A simple DFT calculation:** basic idea about the popular DFT codes, geometry optimization, K-point sampling, pseudopotentials, various DFT functionals and their use (L10+T2) **Applications of DFT-based simulations** (i) electronic structure calculations (band structure, density of states) with examples, bulk modulus, optical and magnetic properties calculations. (ii) DFT-based computational materials design for device applications, surface science, photo- and electro-catalysts, chemical processes of industrial importance (L10+T8).					
Text Book	1. Density Functional Theory: A Practical Introduction, D. Sholl & J. Steckel, Wiley 2009					
Reference Books	1. Electronic Structure – Basic Theory and Practical Methods, R. Martin, Cambridge University Press 2004. 2. Introduction to Solid State Physics, Charles Kittel, Wiley 2004					